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Numerical Analyses for Treating Diffusion in Single-, Two-, and Three-Phase Binary Alloy Systems

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SUMMARY

Finite-difference solutions were developed for treating one-dimensional transient diffusion in single-, two-, and three-phase binary alloy systems. These solutions are applicable for planar, cylindrical, or spherical geometries with any diffusion-zone size and any continuous (within each phase) variation of the diffusion coefficient with concentration. Special techniques were included to account for differences in molal volumes, initiation and growth of an intermediate phase (three-phase system), disappearance of a phase (two- and three-phase systems), and the presence of an initial composition profile in the specimen. In each analysis, an effort was made to achieve good accuracy while minimizing computation time. A major improvement in solution accuracy was achieved in the two-phase analysis by employing a mass-conservation criterion to establish the location of the interface rather than the conventional interface-flux-balance criterion. In the three-phase analysis, computation time was minimized without sacrificing solution accuracy by treating the three-phase problem as a two-phase problem when the thickness of the intermediate phase was less than a preset small value. The computation time was also minimized, without a significant loss of accuracy, by increasing the grid size for longer diffusion times when the concentration in each phase was relatively uniform. For the single-phase analysis, this was accomplished by reducing the number of grid stations with diffusion time. For the two- and three-phase analyses, the grid stations were initially concentrated near the interface, and the zone of analysis was expanded with diffusion time. Comparisons with other solutions were made where possible.

INTRODUCTION

Solutions of the diffusion equation have been reported (refs. 1 to 7) for several different initial and boundary conditions. Most of these, however, are restricted to one geometry, applicable only for infinite or semi-infinite systems, or require that the diffusion coefficient (D) be constant. Heckel and coworkers (refs. 1 to 3) developed finite-difference solutions for two- and three-phase binary alloy systems capable of treating different geometries and any diffusion-zone size, but they assumed D to be a constant. Unnam and Houska (refs. 4 and 5) have reported iterative solutions for single- and two-phase systems allowing for variation of D with concentration, but these solutions were restricted to planar geometry. Finite-difference solutions for single-phase (ref. 6) and two-phase (ref. 7) binary alloy systems allowing for a concentration-dependent D have been reported. However, these solutions were developed only for cylindrical geometry. The computer codes for even these restricted solutions have not, in general, been made available. Therefore, a need exists for more general solutions and their computer codes.

The purpose of this report is to describe general finite-difference solutions for single-, two-, and three-phase binary alloy systems which can treat

one-dimensional diffusion in planar, cylindrical, or spherical geometry specimens with any diffusion-zone size and any concentration dependence of the diffusion coefficient. General computer codes were developed to perform these analyses and are available from COSMIC (refs. 8, 9, and 10). Also available with each code are documentation describing the code, a program listing, and a sample case illustrating typical input and output information. The special features of each analysis are discussed in this report, and example cases are presented to illustrate the validity of the solutions.

SYMBOLS

A,B	elements which constitute binary alloy system
C	composition, atomic fraction of B
$\bar{C}$	average composition for sample, atomic fraction of B
C'	initial concentration of β -phase, assumed to be unity in this study, atomic fraction of B
C ₀	initial concentration of α -phase, assumed to be zero in this study, atomic fraction of B
D	chemical diffusion coefficient, m ² /s
D ^A	chemical diffusion coefficient of pure A, m ² /s
D ^B	chemical diffusion coefficient of pure B, m ² /s
$\bar{D}$	normalized diffusion coefficient, $D/D_{\max}$
D _{max}	maximum diffusion coefficient at temperature of interest for entire composition range in sample, m ² /s
I	number of grid stations in β -phase in two-phase system including grid station at $\beta\alpha$ interface
K _n	normalized distance in the γ -phase, see equation (26)
L	total thickness or diameter of specimen, m
ℓ	initial thickness or diameter of B-rich region, m
m	parameter whose value depends on type of geometry: 0 for planar, 1 for cylindrical, and 2 for spherical
N	total number of grid stations
n	parameter denoting finite-difference grid station
R	normalized distance, $r/(L/2)$

r	distance from center of B-rich region; a subscript n denotes the distance to n th finite-difference grid station, m
T	normalized time, $D_{\max}t/(L/2)^2$
t	time, s
α, β	designations for terminal phases rich in A and B, respectively
γ	designation for intermediate phase
$\delta_{\beta\alpha}$	difference between solubility limits of β - and α -phases, $C_{\beta\alpha} - C_{\alpha\beta}$ (other double subscripts have similar meaning), atomic fraction of B
θ_D	temperature of interest, K
$\xi/2$	distance from center of β -phase to $\beta\alpha$ interface in two-phase system, positive superscript designates α side of interface and negative superscript designates β side of interface, m
$\xi_{1/2}$	distance from center of β -phase to $\beta\gamma$ interface in three-phase system, positive superscript designates γ side of interface and negative superscript designates β side of interface, m
$\xi_{2/2}$	distance from center of β -phase to $\gamma\alpha$ interface in three-phase system, positive superscript designates α side of interface and negative superscript designates γ side of interface, m

Superscripts:

j	index of time increment
α	A-rich phase
β	B-rich phase
γ	intermediate phase

Subscripts:

I	grid-station number in β -phase at $\beta\alpha$ interface of two-phase system
I_1	grid-station number in β -phase at $\beta\gamma$ interface of three-phase system
I_2	grid-station number in γ -phase at $\gamma\alpha$ interface in three-phase system
N	N th grid station of finite-difference grid
n	index of grid station of finite-difference grid

Double subscripts $\alpha\beta$, $\beta\alpha$, $\alpha\gamma$, etc., designate concentration or diffusion coefficient at a particular interface. The first letter indicates the phase being referenced and the two letters together indicate the interface being considered. For example, $C_{\alpha\beta}$ denotes the concentration in the α -phase at the $\alpha\beta$ interface.

THEORETICAL DEVELOPMENT

Single-Phase Systems

Diffusion between pure metals A and B which belong to a single-phase binary alloy system will result in a continuous composition variation of the form shown in figure 1(a). Diffusion in this system can be described by one-dimensional Fick's second law

$$\frac{\partial C}{\partial t} = \frac{1}{r^m} \frac{\partial}{\partial r} \left(r^m D \frac{\partial C}{\partial r} \right) \quad (1)$$

where C is the atomic fraction of B, r is the distance from the center of the B-rich region, D is the concentration-dependent diffusion coefficient, and $m = 0, 1$, or 2 for planar, cylindrical, or spherical geometries, respectively. The initial and boundary conditions to be satisfied are

$$C = C' \quad (0 \leq r < \ell/2; \quad t = 0)$$

$$C = C_0 \quad (\ell/2 < r \leq L/2; \quad t = 0)$$

$$\frac{\partial C}{\partial r} = 0 \quad (r = 0 \quad \text{and} \quad L/2; \quad t \geq 0)$$

where C' and C_0 are the initial compositions of the B-rich and A-rich alloys joined to form the diffusion couple, ℓ is the initial thickness or diameter of the B-rich region, and L is the total thickness or diameter of the specimen.

The finite-difference expression (explicit form, second-order central difference) for Fick's second law is given by

$$\begin{aligned} \frac{C_n^{j+1} - C_n^j}{\Delta t} = D_n^j \left[\frac{m}{r} \left(\frac{C_{n+1}^j - C_{n-1}^j}{2 \Delta r} \right) + \left(\frac{C_{n+1}^j - 2C_n^j + C_{n-1}^j}{(\Delta r)^2} \right) \right] \\ + \left(\frac{C_{n+1}^j - C_{n-1}^j}{2 \Delta r} \right) \left(\frac{D_{n+1}^j - D_{n-1}^j}{2 \Delta r} \right) \end{aligned} \quad (2)$$

For $r = 0$ ($n = 1$), the finite-difference expression is given by

$$\frac{C_1^{j+1} - C_1^j}{\Delta t} = 2(m + 1) D_1^j \left(\frac{C_2^j - C_1^j}{(\Delta r)^2} \right) \quad (3)$$

To obtain this expression, a second-order forward difference was used, and the singularity in the differential equation (eq. (1) for $m = 1$ or 2) at $r = 0$ was taken into account (ref. 11). At $r = L/2$ ($n = N$), equation (2) reduces to

$$\frac{C_N^{j+1} - C_N^j}{\Delta t} = 2D_N^j \left(\frac{C_{N-1}^j - C_N^j}{(\Delta r)^2} \right) \quad (4)$$

The j superscripts designate time increments and the n subscripts designate grid stations in the diffusion couple.

Finite-difference calculations were made by choosing the grid spacing small enough to give convergent solutions of acceptable accuracy. Because explicit formulation was used in the development of the equations, the time increment Δt was selected according to the stability requirement,

$$\Delta t \leq 0.25 \frac{(\Delta r)^2}{D_{\max}} \quad (5)$$

where $D_{\max}$ is the maximum diffusion coefficient for the system at the temperature of interest.

A computer code was developed to solve equations (2) to (5) for any binary alloy system which exhibits complete solid solubility. The FORTRAN IV code, documentation describing the code, and a sample case illustrating typical input and output information are available from COSMIC (ref. 8). The special features of the analysis included in this code are discussed in a subsequent section.

Two-Phase Systems

Diffusion between pure metals which form a two-phase binary alloy system will result in a composition variation between the two metals of the form shown in figure 1(b). The concentrations at the $\alpha\beta$ interface correspond to the equilibrium solubility limits of the β -phase ($C_{\beta\alpha}$) and the α -phase ($C_{\alpha\beta}$) at the temperature θ_D of interest.

Diffusion in a two-phase system can be described by two partial differential equations (Fick's second law for each phase) and an interface-flux-balance equation which describes motion of the interface. The interface-flux-balance equation is given by

$$(C_{\beta\alpha} - C_{\alpha\beta}) \frac{d(\xi/2)}{dt} = D_{\alpha\beta} \left(\frac{dC^\alpha}{dr} \right)_{r=\xi^+/2} - D_{\beta\alpha} \left(\frac{dC^\beta}{dr} \right)_{r=\xi^-/2} \quad (6)$$

where $\xi/2$ is the location of the $\alpha\beta$ interface, with superscripts $+$ and $-$ designating the α and β sides of the interface, respectively. The initial and boundary conditions to be satisfied are

$$C = C' \quad (0 \leq r < l/2; \quad t = 0)$$

$$C = C_0 \quad (l/2 < r \leq L/2; \quad t = 0)$$

$$\frac{\partial C}{\partial r} = 0 \quad (r = 0 \text{ and } L/2; t \geq 0)$$

$$C = C_{\beta\alpha} \quad (r = \xi^-/2)$$

$$C = C_{\alpha\beta} \quad (r = \xi^+/2)$$

In general, the thicknesses of the α - and β -phases change with diffusion time. To account for these dimensional changes, the variable-grid technique developed by Murray and Landis (ref. 12) was used. The number of stations in each phase was held constant and the grid sizes Δr^α and Δr^β changed with time. The β -phase was divided into $I - 1$ equally sized space increments of thickness Δr^β . The α -phase was divided into $N - I - 1$ increments of thickness Δr^α . Two grid stations were located at the interface, one corresponding to the β -phase and the other to the α -phase. The rate of travel of the n th grid point is related to the velocity of the interface by

$$\frac{dr_n}{dt} = \frac{r_n}{\xi/2} \frac{d(\xi/2)}{dt} \quad (7)$$

for the n th point in the β -phase, or by

$$\frac{dr_n}{dt} = \left(\frac{L/2 - r_n}{L/2 - \xi/2} \right) \frac{d(\xi/2)}{dt} \quad (8)$$

for the n th point in the α -phase. The rate of change of concentration at any internal station can be expressed as

$$\frac{dC_n}{dt} = \frac{\partial C_n}{\partial r_n} \frac{dr_n}{dt} + \frac{\partial C_n}{\partial t} \quad (9)$$

where $\partial C_n / \partial t$ is given by equation (1). By combining equations (7) and (9), an expression for the variation of concentration with time at the n th internal station in the β -phase can be written as follows:

$$\frac{dC_n}{dt} = \frac{r_n}{(\xi/2)} \frac{\partial C_n}{\partial r_n} \frac{d(\xi/2)}{dt} + \frac{\partial C_n}{\partial t} \quad (10)$$

In an analogous fashion,

$$\frac{dC_n}{dt} = \left(\frac{L/2 - r_n}{L/2 - \xi/2} \right) \frac{\partial C_n}{\partial r_n} \frac{d(\xi/2)}{dt} + \frac{\partial C_n}{\partial t} \quad (11)$$

gives the change in concentration with time at the n th internal station in the α -phase.

These equations can be normalized by the following change of variables:

$$R_n = \frac{r_n}{L/2} \quad T = \frac{D_{\max} t}{(L/2)^2} \quad \bar{D}_n = \frac{D_n}{D_{\max}}$$

By using these variables, equations (10), (11), (1), and (6) were rewritten as

β -phase:

$$\frac{dC_n}{dT} = \frac{R_n}{\xi/L} \frac{\partial C_n}{\partial R_n} \frac{d(\xi/L)}{dT} + \frac{\partial C_n}{\partial T} \quad (12)$$

α -phase:

$$\frac{dC_n}{dT} = \left(\frac{1 - R_n}{1 - \xi/L} \right) \frac{\partial C_n}{\partial R_n} \frac{d(\xi/L)}{dT} + \frac{\partial C_n}{\partial T} \quad (13)$$

where

$$\frac{\partial C_n}{\partial T} = \bar{D}_n \left(\frac{m}{R_n} \frac{\partial C_n}{\partial R_n} + \frac{\partial^2 C_n}{\partial R_n^2} \right) + \frac{\partial \bar{D}_n}{\partial R_n} \frac{\partial C_n}{\partial R_n} \quad (14)$$

$$\frac{d(\xi/L)}{dT} = \frac{1}{\delta_{\beta\alpha}} \left[\bar{D}_{\alpha\beta} \left(\frac{dC^\alpha}{dR} \right)_{R=\xi^+/L} - \bar{D}_{\beta\alpha} \left(\frac{dC^\beta}{dR} \right)_{R=\xi^-/L} \right] \quad (15)$$

The symbol $\delta_{\beta\alpha}$ denotes the difference between the solubility limits of β - and α -phases.

Equations (12) to (14) were rewritten in finite-difference notation (explicit form, second-order central difference) as follows:

β -phase:

$$\frac{C_n^{j+1} - C_n^j}{\Delta T} = \frac{R_n}{\xi/L} \frac{d(\xi/L)}{dT} \left(\frac{C_{n+1}^j - C_{n-1}^j}{2 \Delta R^\beta} \right) + \frac{\partial C_n}{\partial T} \quad (16)$$

α -phase:

$$\frac{C_n^{j+1} - C_n^j}{\Delta T} = \left(\frac{1 - R_n}{1 - \xi/L} \right) \left(\frac{C_{n+1}^j - C_{n-1}^j}{2 \Delta R^\alpha} \right) \frac{d(\xi/L)}{dT} + \frac{\partial C_n}{\partial T} \quad (17)$$

where

$$\begin{aligned} \frac{\partial C_n}{\partial T} = \bar{D}_n^j & \left[\frac{m}{R_n} \left(\frac{C_{n+1}^j - C_{n-1}^j}{2 \Delta R} \right) + \left(\frac{C_{n+1}^j - 2C_n^j + C_{n-1}^j}{(\Delta R)^2} \right) \right] \\ & + \left(\frac{\bar{D}_{n+1}^j - \bar{D}_{n-1}^j}{2 \Delta R} \right) \left(\frac{C_{n+1}^j - C_{n-1}^j}{2 \Delta R} \right) \end{aligned} \quad (18)$$

The finite-difference expression (second-order forward and reverse difference) for the interface-flux-balance equation (15) is

$$\frac{(\xi/L)^{j+1} - (\xi/L)^j}{\Delta T} = \frac{1}{\delta_{\beta\alpha}} \left[\bar{D}_{\alpha\beta} \left(\frac{-C_{I+3}^j + 4C_{I+2}^j - 3C_{\alpha\beta}^j}{2 \Delta R^\alpha} \right) - \bar{D}_{\beta\alpha} \left(\frac{C_{I-2}^j - 4C_{I-1}^j + 3C_{\beta\alpha}^j}{2 \Delta R^\beta} \right) \right] \quad (19)$$

The finite-difference expressions for the boundary conditions are given by

$$\frac{C_1^{j+1} - C_1^j}{\Delta T} = 2(m+1) \bar{D}_1^j \left(\frac{C_2^j - C_1^j}{(\Delta R^\beta)^2} \right) \quad (R = 0) \quad (20)$$

$$\frac{C_N^{j+1} - C_N^j}{\Delta T} = 2 \bar{D}_N^j \left(\frac{C_{N-1}^j - C_N^j}{(\Delta R^\alpha)^2} \right) \quad (R = 1) \quad (21)$$

To perform the finite-difference calculations, the grid spacing ΔR must be chosen small enough to give convergent solutions of acceptable accuracy. Also, because explicit formulation was used in the development of the equations, the time increment ΔT must be selected according to the stability requirement (similar to eq. (5)),

$$\Delta T_{\max} \leq 0.25(\Delta R_{\min})^2 \quad (22)$$

where $\Delta T_{\max}$ is the maximum time increment and $\Delta R_{\min}$ is the minimum grid spacing.

A computer code was developed to solve equations (16) to (22) for any two-phase binary alloy system. The FORTRAN IV code, documentation describing the code, and a sample case illustrating typical input and output information are available from COSMIC (ref. 9). The special features of the analysis included in this code are discussed in a subsequent section.

Three-Phase Systems

Diffusion between pure metals which form a two-phase binary alloy system with an intermediate phase will result in a composition variation between the two metals of the form shown in figure 1(c). The concentrations at the $\beta\gamma$ interface correspond to the equilibrium solubility limits of the β -phase ($C_{\beta\gamma}$) and the γ -phase ($C_{\gamma\beta}$) at the temperature of interest. The concentrations at the $\gamma\alpha$ interface correspond to the equilibrium solubility limits of the γ -phase ($C_{\gamma\alpha}$) and the α -phase ($C_{\alpha\gamma}$).

Diffusion in this system can be described by Fick's second law for each phase and two interface-flux-balance equations. The interface-flux-balance equations are of the form

$$(C_{\beta\gamma} - C_{\gamma\beta}) \frac{d(\xi_1/2)}{dt} = D_{\gamma\beta} \left(\frac{dC^\gamma}{dr} \right)_{r=\xi_1^+/2} - D_{\beta\gamma} \left(\frac{dC^\beta}{dr} \right)_{r=\xi_1^-/2} \quad (23)$$

at the $\beta\gamma$ interface and

$$(C_{\gamma\alpha} - C_{\alpha\gamma}) \frac{d(\xi_2/2)}{dt} = D_{\alpha\gamma} \left(\frac{dC^\alpha}{dr} \right)_{r=\xi_2^+/2} - D_{\gamma\alpha} \left(\frac{dC^\gamma}{dr} \right)_{r=\xi_2^-/2} \quad (24)$$

at the $\gamma\alpha$ interface, where $\xi_1/2$ is the location of the $\beta\gamma$ interface with superscripts + and - denoting the γ and β sides of the interface, respectively, and $\xi_2/2$ is the location of the $\gamma\alpha$ interface with superscripts + and - denoting the α and γ sides of the interface, respectively. The initial and boundary conditions to be satisfied are

$$C = C' \quad (0 \leq r < l/2; \quad t = 0)$$

$$C = C_0 \quad (l/2 < r \leq L/2; \quad t = 0)$$

$$\frac{\partial C}{\partial r} = 0 \quad (r = 0 \quad \text{and} \quad L/2; \quad t \geq 0)$$

All interface concentrations are assumed equal to the equilibrium solubility limits of the phases:

$\beta\gamma$ interface:

$$C = C_{\beta\gamma} \quad (r = \xi_1^-/2)$$

$$C = C_{\gamma\beta} \quad (r = \xi_1^+/2)$$

$\gamma\alpha$ interface:

$$C = C_{\gamma\alpha} \quad (r = \xi_2^-/2)$$

$$C = C_{\alpha\gamma} \quad (r = \xi_2^+/2)$$

In general, the thicknesses of the β -, γ -, and α -phases change with diffusion time. To account for these dimensional changes, the variable-grid finite-difference technique previously discussed for the two-phase analysis was used. The number of grid points in each phase was held constant and the grid sizes Δr^β , Δr^γ , and Δr^α changed with time. The rate of change of concentration at any internal station is given by equation (9) where the velocity of the n th grid point dr_n/dt in each phase is given by

$$\frac{dr_n}{dt} = \frac{r_n}{\xi_1/2} \frac{d(\xi_1/2)}{dt} \quad (25)$$

for the n th point in the β -phase, by

$$\frac{dr_n}{dt} = \frac{d(\xi_1/2)}{dt} + K_n \left[\frac{d(\xi_2/2)}{dt} - \frac{d(\xi_1/2)}{dt} \right] \quad (26)$$

for the nth point in the γ -phase where

$$K_n = \frac{r_n - \xi_{1/2}}{\xi_{2/2} - \xi_{1/2}}$$

and by

$$\frac{dr_n}{dt} = \left(\frac{L/2 - r_n}{L/2 - \xi_{2/2}} \right) \frac{d(\xi_{2/2})}{dt} \quad (27)$$

for the nth point in the α -phase. The equations for the rate of change of concentration at any internal station in the three phases are obtained by substituting equations (25), (26), and (27) into equation (9):

β -phase:

$$\frac{dC_n}{dt} = \frac{r_n}{\xi_{1/2}} \frac{d(\xi_{1/2})}{dt} \frac{\partial C_n}{\partial r_n} + \frac{\partial C_n}{\partial t} \quad (28)$$

γ -phase:

$$\frac{dC_n}{dt} = \left\{ \frac{d(\xi_{1/2})}{dt} + K_n \left[\frac{d(\xi_{2/2})}{dt} - \frac{d(\xi_{1/2})}{dt} \right] \right\} \frac{\partial C_n}{\partial r_n} + \frac{\partial C_n}{\partial t} \quad (29)$$

α -phase:

$$\frac{dC_n}{dt} = \left(\frac{L/2 - r_n}{L/2 - \xi_{2/2}} \right) \frac{d(\xi_{2/2})}{dt} \frac{\partial C_n}{\partial r_n} + \frac{\partial C_n}{\partial t} \quad (30)$$

Normalizing the distance, time, and diffusion coefficient in the same manner as was done previously for the two-phase analysis reduces equations (28) to (30) to

β -phase:

$$\frac{dC_n}{dT} = \frac{R_n}{\xi_{1/L}} \frac{d(\xi_{1/L})}{dT} \frac{\partial C_n}{\partial R_n} + \frac{\partial C_n}{\partial T} \quad (31)$$

γ -phase:

$$\frac{dC_n}{dT} = \left\{ \frac{d(\xi_{1/L})}{dT} + K_n \left[\frac{d(\xi_{2/L})}{dT} - \frac{d(\xi_{1/L})}{dT} \right] \right\} \frac{\partial C_n}{\partial R_n} + \frac{\partial C_n}{\partial T} \quad (32)$$

α -phase:

$$\frac{dC_n}{dT} = \left(\frac{1 - R_n}{1 - \xi_{2/L}} \right) \frac{d(\xi_{2/L})}{dT} \frac{\partial C_n}{\partial R_n} + \frac{\partial C_n}{\partial T} \quad (33)$$

where $\partial C_n / \partial T$ is given by equation (14). Likewise, the interface-flux-balance equations (23) and (24) can be rewritten as

$\beta\gamma$ interface:

$$\frac{d(\xi_1/L)}{dT} = \frac{1}{\delta_{\beta\gamma}} \left[\bar{D}_{\gamma\beta} \left(\frac{dC^\gamma}{dR} \right)_{R=\xi_1^+/L} - \bar{D}_{\beta\gamma} \left(\frac{dC^\beta}{dR} \right)_{R=\xi_1^-/L} \right] \quad (34)$$

$\gamma\alpha$ interface:

$$\frac{d(\xi_2/L)}{dT} = \frac{1}{\delta_{\gamma\alpha}} \left[\bar{D}_{\alpha\gamma} \left(\frac{dC^\alpha}{dR} \right)_{R=\xi_2^+/L} - \bar{D}_{\gamma\alpha} \left(\frac{dC^\gamma}{dR} \right)_{R=\xi_2^-/L} \right] \quad (35)$$

where

$$\delta_{\beta\gamma} = C_{\beta\gamma} - C_{\gamma\beta}$$

$$\delta_{\gamma\alpha} = C_{\gamma\alpha} - C_{\alpha\gamma}$$

Equations (31) to (35) can be expressed in finite-difference notation in a manner analogous to that discussed for two-phase systems:

β -phase:

$$\frac{C_n^{j+1} - C_n^j}{\Delta T} = \frac{R_n}{\xi_1/L} \frac{d(\xi_1/L)}{dT} \left(\frac{C_{n+1}^j - C_{n-1}^j}{2 \Delta R^\beta} \right) + \frac{\partial C_n}{\partial T} \quad (36)$$

γ -phase:

$$\frac{C_n^{j+1} - C_n^j}{\Delta T} = \left\{ \frac{d(\xi_1/L)}{dT} + K_n \left[\frac{d(\xi_2/L)}{dT} - \frac{d(\xi_1/L)}{dT} \right] \right\} \left(\frac{C_{n+1}^j - C_{n-1}^j}{2 \Delta R^\gamma} \right) + \frac{\partial C_n}{\partial T} \quad (37)$$

α -phase:

$$\frac{C_n^{j+1} - C_n^j}{\Delta T} = \left(\frac{1 - R_n}{1 - \xi_2/L} \right) \frac{d(\xi_2/L)}{dT} \left(\frac{C_{n+1}^j - C_{n-1}^j}{2 \Delta R^\alpha} \right) + \frac{\partial C_n}{\partial T} \quad (38)$$

where $\partial C_n / \partial T$ is given by equation (18). The finite-difference expressions for the interface-flux-balance equations (34) and (35) are

$\beta\gamma$ interface:

$$\begin{aligned} \frac{(\xi_1/L)^{j+1} - (\xi_1/L)^j}{\Delta t} = & \frac{1}{\delta_{\beta\gamma}} \left[\bar{D}_{\gamma\beta} \left(\frac{-C_{I1+3}^j + 4C_{I1+2}^j - 3C_{\gamma\beta}^j}{2 \Delta R^\gamma} \right) \right. \\ & \left. - \bar{D}_{\beta\gamma} \left(\frac{C_{I1-2}^j - 4C_{I1-1}^j + 3C_{\beta\gamma}^j}{2 \Delta R^\beta} \right) \right] \end{aligned} \quad (39)$$

$\gamma\alpha$ interface:

$$\frac{(\xi_{2/L})^{j+1} - (\xi_{2/L})^j}{\Delta T} = \frac{1}{\delta_{\gamma\alpha}} \left[\bar{D}_{\alpha\gamma} \left(\frac{-C_{I2+3}^j + 4C_{I2+2}^j - 3C_{\alpha\gamma}^j}{2 \Delta R^\alpha} \right) - \bar{D}_{\gamma\alpha} \left(\frac{C_{I2-2}^j - 4C_{I2-1}^j + 3C_{\gamma\alpha}^j}{2 \Delta R^\gamma} \right) \right] \quad (40)$$

The finite-difference expressions for the boundaries are given by equations (20) and (21).

The grid spacing ΔR was chosen small enough to give convergent solutions of acceptable accuracy, and the time increment was chosen according to the same stability requirement that was used for the two-phase system (eq. (22)).

A computer code was developed to solve equations (18), (20) to (22), and (36) to (40). The FORTRAN IV code, documentation describing the code, and a sample case illustrating typical input and output information are available from COSMIC (ref. 10). The special features of the analysis included in this code are discussed in the following section.

SPECIAL FEATURES OF ANALYSES

Single-Phase Analysis

Volume change.— To account for volume changes which occur during diffusion due to differences in the molal volumes of the pure metals, the concentration was expressed in terms of the volume fraction of one of the diffusing components. All concentrations were converted into volume fraction for the calculations and then converted back to atomic fraction once the desired solution had been obtained.

Logarithmic interpolation of D .— Logarithmic interpolation of the concentration-dependent diffusion coefficient was employed in the analysis because of the general trend for $\log D$ to vary linearly with C for several binary alloy systems (ref. 13).

Initial composition profile.— Two optional initial conditions were treated: (1) no prior diffusion between the A-rich and B-rich regions, and (2) prior diffusion resulting in a concentration gradient across the interface region. Most analyses treat the case of no prior diffusion where both regions of the couple are uniform in composition with a sharp change in composition at the interface. The second option, however, allows an experimentally determined concentration profile to be treated as the initial condition to calculate how much more diffusion will occur with additional exposure at elevated temperature. This feature was added because in the consolidation of many metal-matrix composites, some diffusion occurs between fibers (or particles) and the matrix.

Finite-difference grid size.— For long diffusion times, one or more grid changes were made to reduce the total number of grid stations to a minimum (20)

in an effort to minimize computer time. The concentrations corresponding to each new grid point were determined by interpolation between points on the old grid.

Two-Phase Analysis

Differences in molal volumes, concentration dependence of the diffusion coefficient, and the presence of an initial concentration profile in the sample were accounted for by using the procedures previously discussed for single-phase systems.

Finite-difference grid size.- To improve solution accuracy, grid stations were concentrated near the interface during the initial stages of diffusion when the diffusion zone was small relative to the specimen dimensions. When the concentrations at the outer bounds of the zone being analyzed began to change, the zone size was enlarged. In general, two or three zone expansions were performed before the bounds of the α - and β -phases were reached. In all cases, the number of grid stations in each phase was held constant. After each expansion of the zone, the concentrations at the new grid locations were determined by interpolation from the concentration profile (present in the specimen) just prior to expanding the zone.

Interface-location criteria.- For the two-phase system, solution accuracy was improved by (1) employing an iterative mass-conservation procedure to locate the $\alpha\beta$ interface rather than relying on the interface-flux-balance relationship and (2) using logarithmic average diffusion coefficients at the interface rather than the diffusion coefficients corresponding to the concentrations at the interface. Both of these changes compensate for numerical approximation errors inherent in the procedure used to calculate the interface concentration gradients.

Logarithmic average interface diffusion coefficients were calculated by the expressions

$$\bar{D}_{\alpha\beta} = \sqrt{\bar{D}_{I+1}\bar{D}_{I+2}}$$

$$\bar{D}_{\beta\alpha} = \sqrt{\bar{D}_{I-1}\bar{D}_I}$$

where $\bar{D}_{\alpha\beta}$ and $\bar{D}_{\beta\alpha}$ are the normalized diffusion coefficients used in equation (19).

The iterative mass-conservation procedure consisted of solving the interface-flux-balance equation (eq. (19)) to obtain an estimate of the location of the $\alpha\beta$ interface and adjusting this location in the positive or negative direction to force the system to conserve. This refined interface location was used to calculate new grid spacings ΔR^α and ΔR^β which in turn were used to calculate new grid-point locations. The concentrations at the new grid points were assumed equal to the concentrations at the old grid points before shifting the interface. The mass-conservation procedure was repeated to obtain a further refinement in the interface location. In general, only two or three iterations were required to establish convergence.

Phase-termination criteria.- For all β -phase concentrations less than $C_{\beta\alpha} + 10^{-6}$, $\Delta R_{\min}$ in the stability criterion (eq. (22)) was taken as ΔR^{α} , and the β -phase concentrations were not computed from this time onward. In an analogous fashion, the α -phase concentrations were not computed if all the α -phase concentrations were greater than $C_{\alpha\beta} - 10^{-6}$. If both conditions were met, or if the β -phase thickness was 0.01 of its initial thickness, no further calculations were performed.

Three-Phase Analysis

To account for differences in molal volumes, concentration dependence of the diffusion coefficient, and the presence of an initial concentration profile in the three-phase system, the procedures previously discussed for single-phase systems were employed. As previously discussed for the two-phase analysis, grid stations were concentrated near the interface during early stages of diffusion, and the zone of analysis was expanded with diffusion time.

Initiation and growth of intermediate phase.- Initiation of the intermediate phase (γ) was treated by assuming that γ was initially present in the sample in the form of a thin (0.05 μm) layer between the α - and β -phases. The concentration gradient in γ was assumed to vary linearly between the solubility limits $C_{\gamma\beta}$ and $C_{\gamma\alpha}$. If D^{γ} was less than D^{α} or D^{β} , the γ -phase remained thin for most or all of the homogenization process depending on the value of the average composition $\bar{C}$ and the solubilities of the α - and β -phases. Under these conditions, a large amount of computation time was required to perform the calculations because the grid size in the γ -phase Δr^{γ} remained small and dictated a very small Δt (eq. (22)). To overcome this problem, the interface-flux-balance equations were solved to determine the thickness change of each phase with time, but compositional changes in the γ -phase were not computed and a linear gradient was assumed. Because γ -phase concentrations were not calculated, the time increment for the finite-difference analysis was determined by the relatively larger grid spacings in the α - or β -phases. This procedure resulted in significant savings in computation time. If the γ -phase thickness grew larger than a small preset value, concentrations in the γ -phase were calculated.

To prevent oscillations in the thickness of the γ -phase, the time increment for the diffusion calculations was selected small enough to limit the thickness change of the γ -phase to no more than 2 percent of its previous value during any one time increment. This was accomplished by calculating Δt for the α - and β -phases and using the smaller of these to calculate the change in thickness of the γ -phase. If the change was more than 2 percent, Δt was reduced to give a 2-percent change in the thickness of the γ -phase.

Phase-termination criteria.- If any phase thickness was less than 1 percent of the total zone thickness, or if all the concentrations within a given phase were within 10^{-6} , the concentrations in that phase were assumed to remain constant during subsequent time increments. Also, the grid spacing in this phase was not used to compute the time increment. If the thickness of any phase was

less than 0.001 percent of the total diffusion-zone thickness, this phase thickness was assumed to be equal to zero.

RESULTS AND DISCUSSION

Mass Conservation

As previously discussed, an iterative mass-conservation procedure was used in the two-phase analysis instead of the conventional interface-flux-balance procedure. Calculations were performed to assess the improvement in solution accuracy resulting from this change. Typical results are shown in figure 2. The conditions selected for this assessment were: cylindrical geometry, $l/2 = 20 \mu\text{m}$, $L/2 = 140 \mu\text{m}$, $C' = 1.0$, $C_{\beta\alpha} = 0.85$, $C_{\alpha\beta} = 0.15$, $C_0 = 0$, and $D^\alpha = D^\beta = 10^{-14} \text{ m}^2/\text{s}$. Solutions were calculated for initial α -phase grid sizes of 0.5, 0.86, 3, and 6 μm and an initial β -phase grid size of 1 μm for all cases. Figure 2(b) compares normalized interface locations at $t = 90\,000 \text{ s}$ calculated by the two interface-location criteria as a function of the initial grid size in the α -phase. Use of mass conservation resulted in a faster rate of convergence as the α -phase grid size was decreased. Very small initial α -phase grid sizes were required to predict the same interface location by both methods. If the flux-balance criterion were used, very small grid sizes are required to give conservation of mass; see figure 2(a). These results suggest that the mass-conservation criterion improves solution accuracy and significantly reduces computation time because a larger grid size can be used.

A mass-conservation criterion cannot readily be used in the three-phase analysis because of the additional complexity associated with the presence of two interfaces. If the system deviates from conservation, no simple way was found to determine how much each interface should be shifted to force the system to conserve.

Intermediate-Phase Growth

The procedure used to treat the initiation and growth of an intermediate phase in the three-phase analysis was previously discussed. If the intermediate phase was thin, the three-phase problem was essentially reduced to a two-phase problem by not calculating the concentrations at the finite-difference grid stations located in the intermediate phase. However, the time increment Δt for the finite-difference calculation was selected small enough that the growth of the intermediate phase was stable. The Δt was chosen so that the thickness of the intermediate phase did not change by more than 2 percent during any time increment. The effectiveness of this procedure is illustrated by the results shown in figure 3. Compared in this figure are γ -phase thicknesses determined with (1) the three-phase calculation, (2) the two-phase calculation using a ± 2 -percent-change criterion to select Δt , and (3) a two-phase calculation using a change criterion of -50 to +100 percent to select Δt . The three-phase calculations and the two-phase calculations with a ± 2 -percent-change criterion converge after approximately 60 s of diffusion time. The two-phase calculation

with the change criterion of -50 to +100 percent was unstable and caused the γ -phase thickness to oscillate about the three-phase results.

For the diffusion conditions selected for this illustration, the computer time required to calculate the solution for 60 s of diffusion time was more than a factor of 100 larger for the three-phase calculation than for the two-phase calculation using the ± 2 -percent-change criterion. Although this time difference was somewhat dependent on the solubilities and diffusion coefficients of each phase, the difference was always large for those cases considered where $D^\gamma < D^\alpha$ or D^β .

Example Cases and Comparisons With Other Solutions

Single-phase analysis.- A comparison of results calculated by the present finite-difference solution and an iterative solution technique (ref. 4) also capable of treating concentration-dependent D is shown in figure 4. In this calculation, D varied linearly on a logarithmic scale with concentration. The D for pure A was assumed to be an order of magnitude larger than the D for pure B. The exposure time was 5 hr and the geometry of the specimen was planar. The iterative solution technique of Unnam and Houska (ref. 4) is applicable only for planar geometry. The excellent agreement between the two solution techniques is typical of that found for all other exposure conditions considered. These results provide a check for the finite-difference analysis developed in this investigation.

Two-phase analysis.- Results of this analysis were compared with those of a closed-form iterative technique reported by Unnam and Houska (ref. 4). Comparable solutions were obtained for a wide range of input parameters for planar interfaces (solution of ref. 4 is valid only for planar interfaces). Several different phase thicknesses and D variations were considered in order to yield information regarding solution stability and accuracy. No significant differences were found between the results obtained from the two solutions. The interface positions calculated by the finite-difference program were always within 5 percent of the positions calculated by the iterative solution.

A comparison was also made with experimentally determined diffusion data on W-Ni laminates reported by Tanzilli and Heckel (ref. 2). They prepared multilayer W-Ni couples with two mean compositions, $\bar{C} = 0.152$ and $\bar{C} = 0.121$ atomic fraction of W. These couples were diffused at 1480 and 1429 K, and then they were sectioned perpendicular to the layers and metallographically polished. The extent of diffusion was determined by measuring the average thickness of the W-rich layers after each exposure. Their results are presented in figure 5 where the normalized thickness of the β -layer, ξ/l , is plotted as a function of a dimensionless time factor, $D^\alpha t/l^2$, where ξ is the β -phase (W-rich) thickness at time t , l is the initial thickness of this layer, and D^α is the concentration-independent diffusion coefficient in the α -phase (Ni-rich). Also plotted on this graph are results obtained from (1) a constant- D finite-difference solution developed by Tanzilli and Heckel (ref. 2), (2) the present variable- D finite-difference solution with the planar geometry option, and (3) the iterative solution developed by Unnam and Houska (ref. 4). For cases (2) and (3), the diffusion-coefficient data of Walsh and Donachie (ref. 14) were

used for the α -phase region and the data of Vasilev and Chernomorchenko (ref. 15) were used for the β -phase region. The same initial and boundary conditions were used in all these solutions. The analytical results are shown only for the sample with $\bar{C} = 0.152$, as the curves were the same for $\bar{C} = 0.152$ or 0.121 until ξ/l dropped below about 0.3. Also, no experimental data points were available below $\xi/l = 0.3$ for the $\bar{C} = 0.121$ sample.

The interface positions calculated by all three solutions agree. The curve obtained from the present analysis best fits the experimental data points.

Three-phase analysis.— To study the effect of large D^α variations on the diffusion process, calculations were performed for D^α/D^β ratios of 1, 100, and 0.01 holding D^β and D^γ constant at 10^{-14} m²/s. Average concentration of the couple was 0.40 atomic fraction of B and the solubility limits were $C' = 1.0$, $C_{\beta\gamma} = 0.99$, $C_{\gamma\beta} = 0.51$, $C_{\gamma\alpha} = 0.49$, $C_{\alpha\gamma} = 0.20$, and $C_0 = 0$. The small solubility range of the β -phase, 0.01, and γ -phase, 0.02, mean that any differences in the diffusion kinetics are predominantly due to differences in diffusion in the α -phase. The normalized thickness of the β - and γ -phases are plotted as a function of $\sqrt{t}$ in figure 6(a). The curves for $D^\alpha = D^\beta = D^\gamma$ provide a basis for comparison of the other two curves. If D^α is small ($D^\alpha/D^\beta = 0.01$), the rate of decrease of the β -phase is slower and the rate of growth of the γ -phase is faster than the corresponding curves for $D^\alpha/D^\beta = 1$. If D^α is high ($D^\alpha/D^\beta = 100$), a rapid loss of β -phase thickness and slow initial growth of the γ -phase occur. At approximately $\sqrt{t} = 50$, the rate of decrease of the β -phase is greatly reduced and the rate of growth of the γ -phase increases. The corresponding concentration profiles (fig. 6(b)) show that these changes are due to the small concentration gradient in the α -phase for the high D^α case. A small gradient in the α -phase implies a small flux into the γ -phase which increases the growth rate of the γ -phase and reduces the rate of loss of the β -phase.

CONCLUDING REMARKS

Finite-difference solutions of the one-dimensional transient diffusion equations describing diffusion in single-, two-, and three-phase binary alloy systems were developed. These solutions are applicable for any diffusion-zone size and for planar, cylindrical, or spherical geometries. Each analysis also treats concentration dependence of the diffusion coefficient. General computer codes were developed to perform each analysis. These computer codes, documentation describing the codes, and sample cases illustrating typical input and output are available from COSMIC. Special features were included in the computer codes to account for differences in molal volumes, initiation and growth of an intermediate phase (three-phase system), disappearance of a phase (two- and three-phase systems), and the presence of an initial composition profile in the specimen. Each computer code was optimized to achieve good accuracy while minimizing computation time. The use of a mass-conservation criterion to locate the interface in the two-phase system rather than the conventional flux-balance criterion resulted in improvement in solution accuracy and reduction in computation time. In the three-phase analysis, computation time was reduced by not performing the concentration calculations in the intermediate phase when that phase was thin. In all three computer codes, the grid spacings were increased during

the later stages of diffusion when the concentration gradients were small. The increased grid spacing allowed increased time increments and thus minimized computation times. In the single-phase analysis, this was accomplished by reducing the number of grid stations with diffusion time. In the two- and three-phase analyses, a given number of grid stations were initially concentrated in a narrow zone near the interface. For longer diffusion times, this zone was expanded until the specimen boundaries were reached.

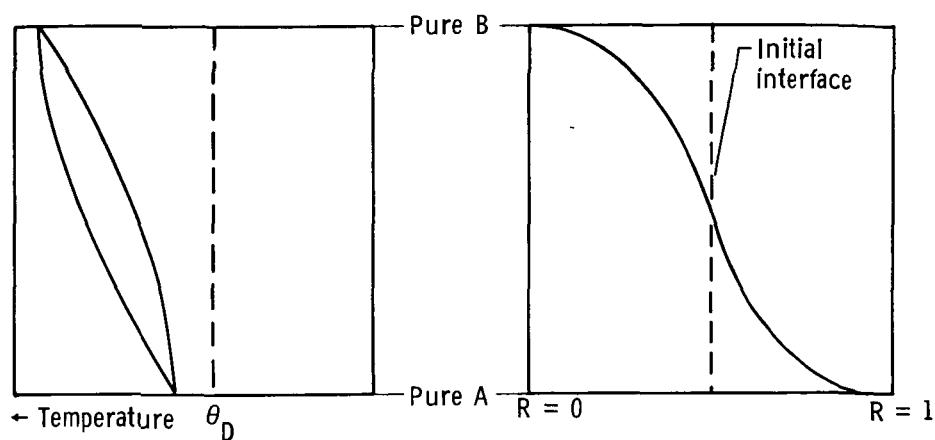
The results of the single- and two-phase analyses were in good agreement with solutions or data reported in the literature for those cases where a direct comparison could be made. A direct comparison of the three-phase results was not possible because neither experimental nor accurate analytical data were available from the literature.

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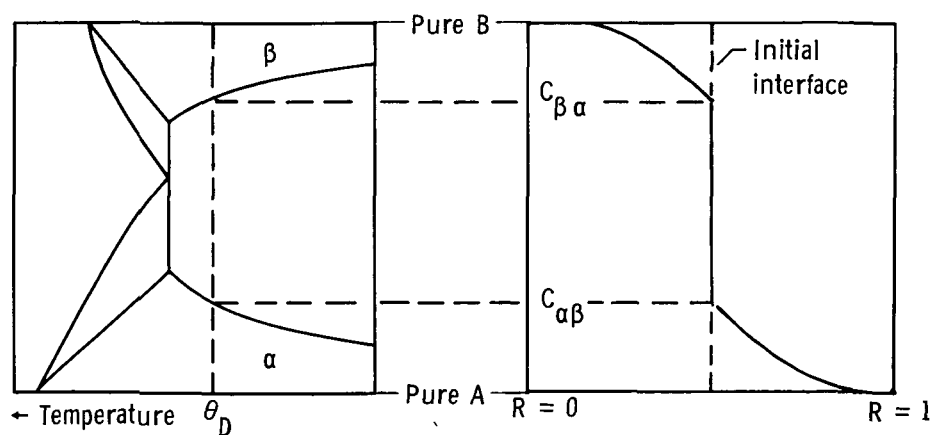
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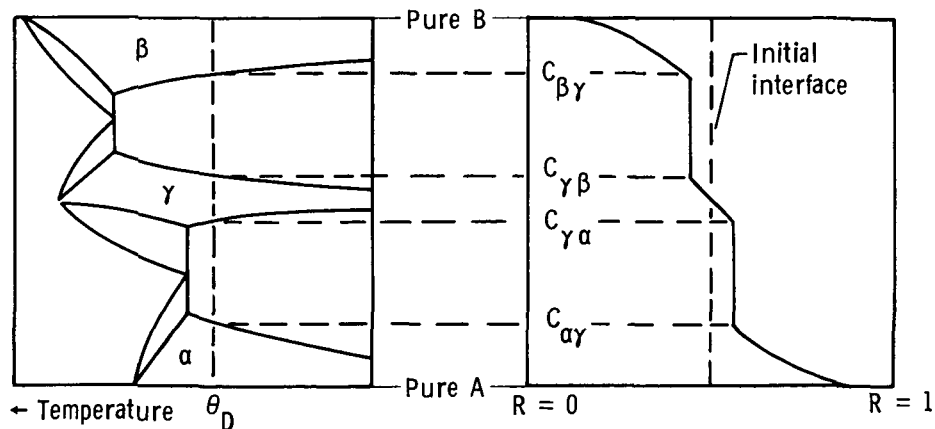
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(a) Single phase - complete solid solubility.

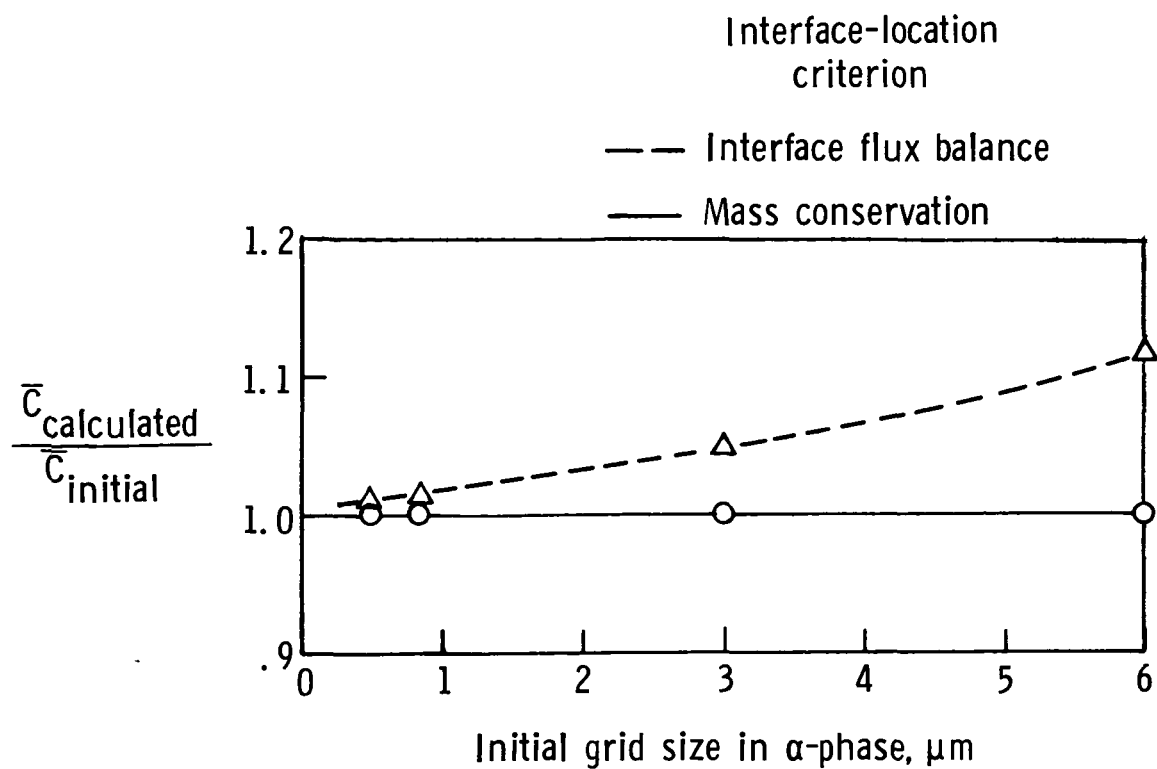


(b) Two phase - limited solid solubility.

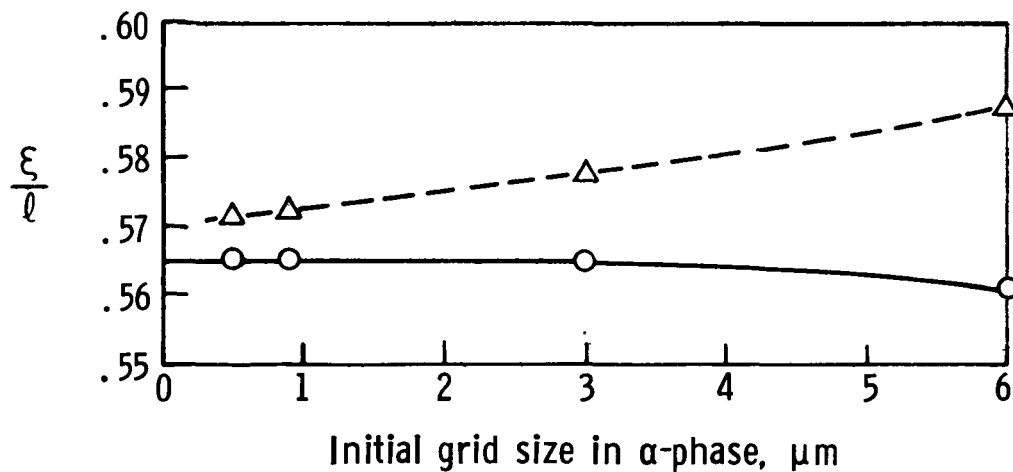


(c) Three phase - intermediate-phase formation.

Figure 1.- Phase diagrams and example concentration profiles produced by diffusion between initially pure A and pure B at temperature θ_D in single-, two-, and three-phase binary alloy systems.



(a) Mass conservation.



(b) Convergence of interface location.

Figure 2.- Effect of interface-location criteria on (a) mass conservation and (b) convergence of interface location for different initial grid sizes in α -phase. Cylindrical geometry.

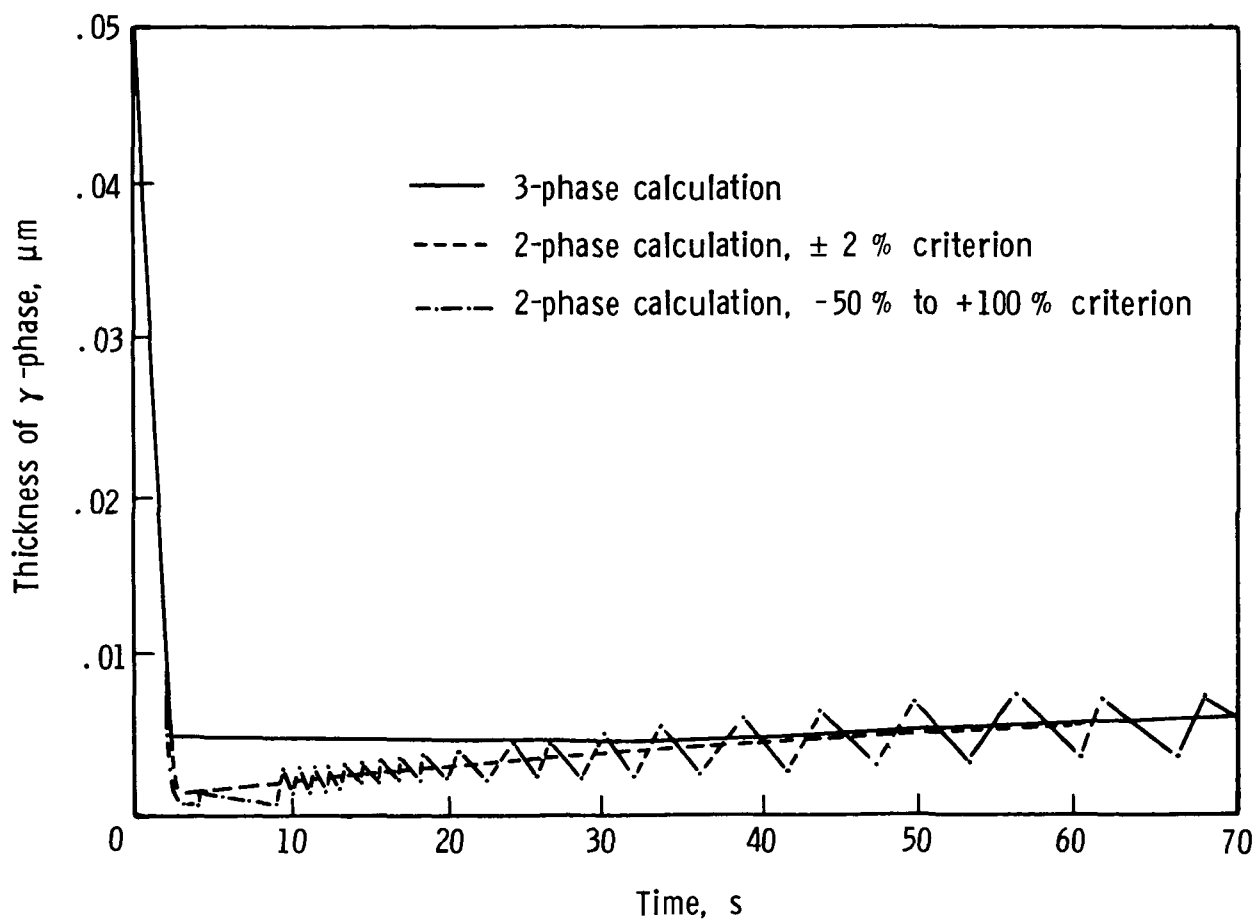


Figure 3.- Accuracy and stability during intermediate-phase (γ) initiation.

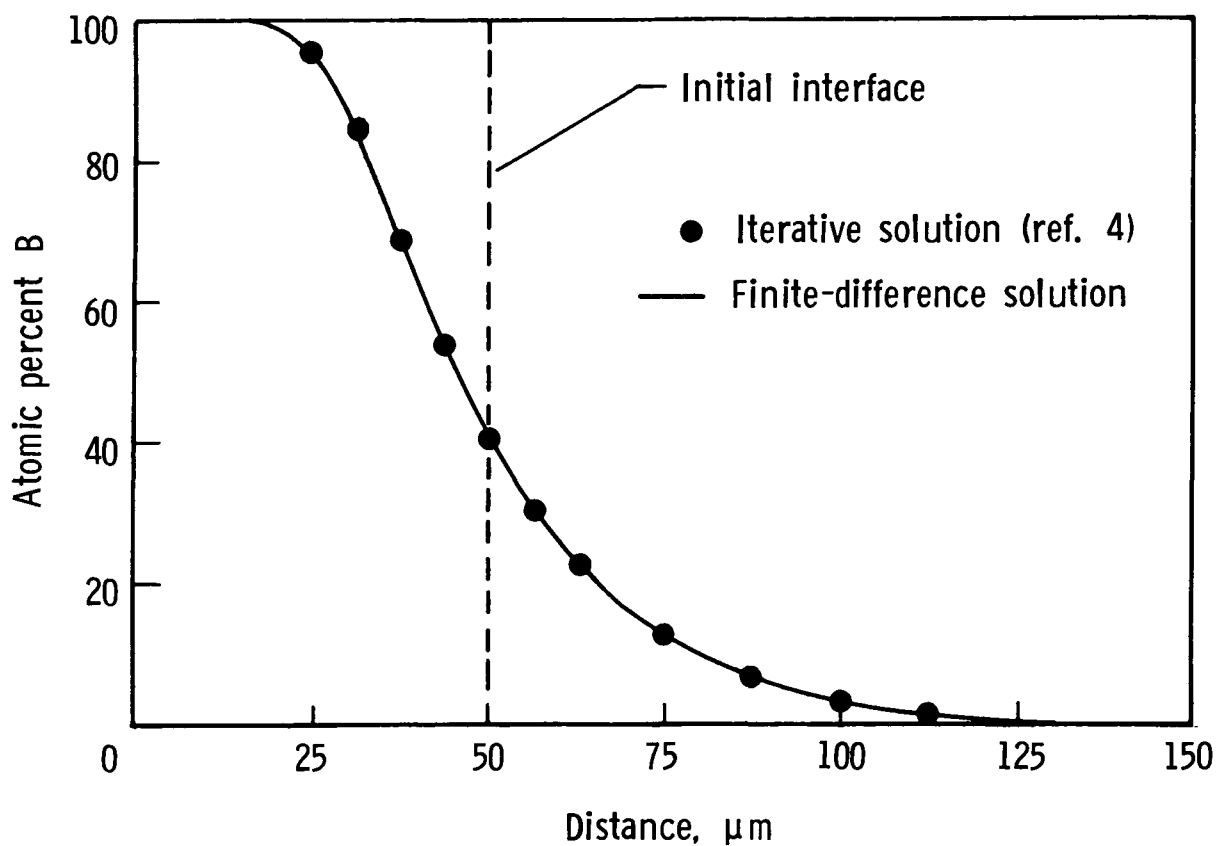


Figure 4.- Comparison of concentration profiles in single-phase system calculated by the present analysis and an iterative solution reported by Unnam and Houska (ref. 4). Planar geometry; $D^A = 10D^B$; $t = 5$ hr.

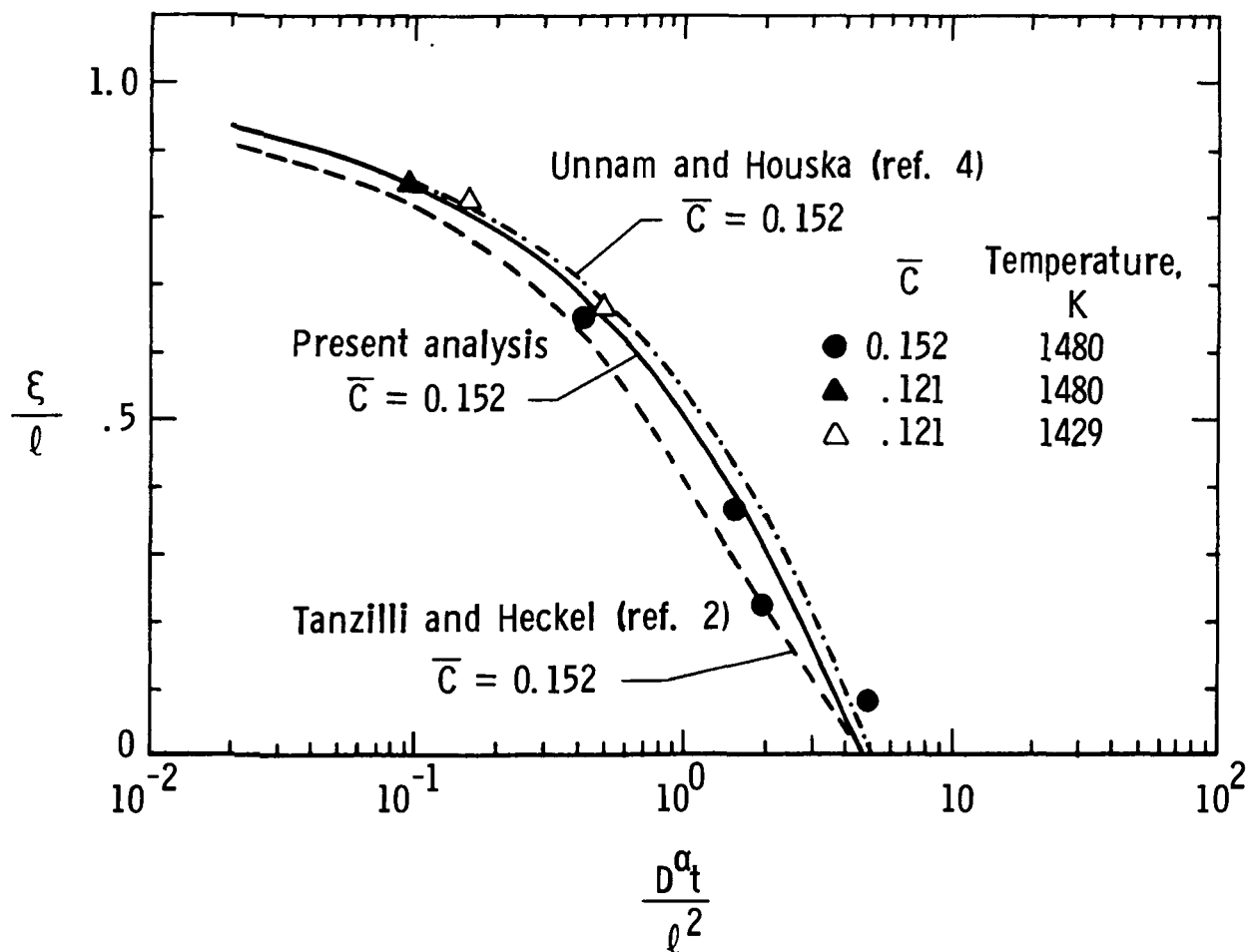
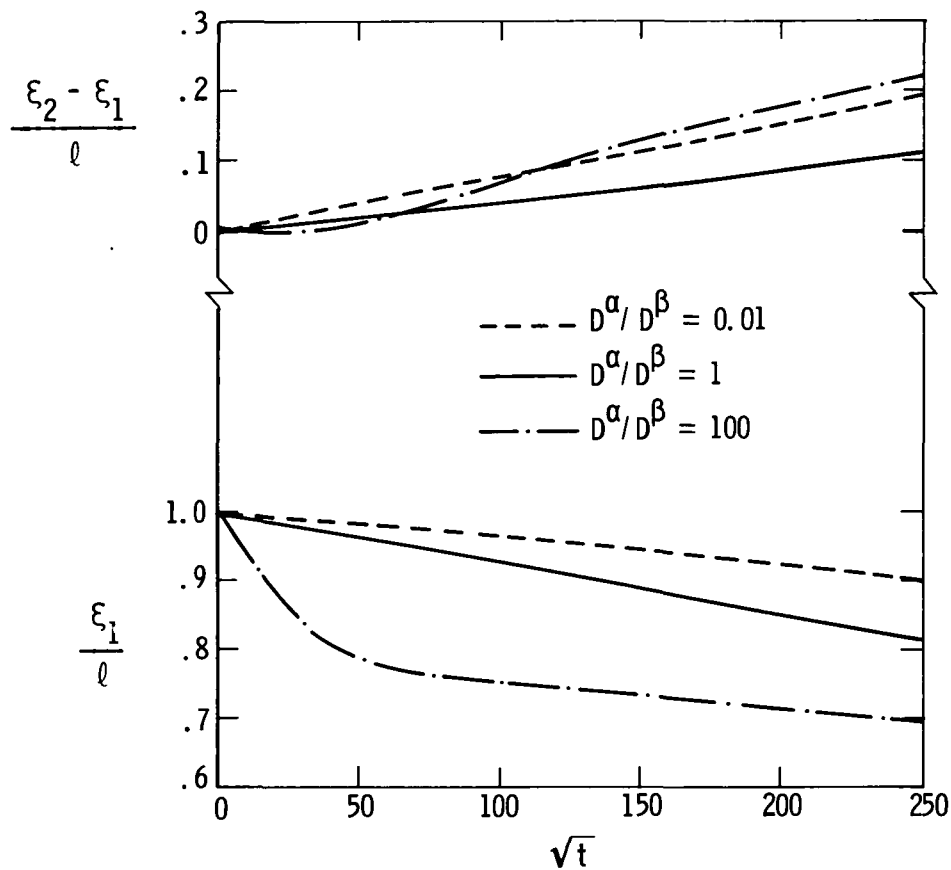
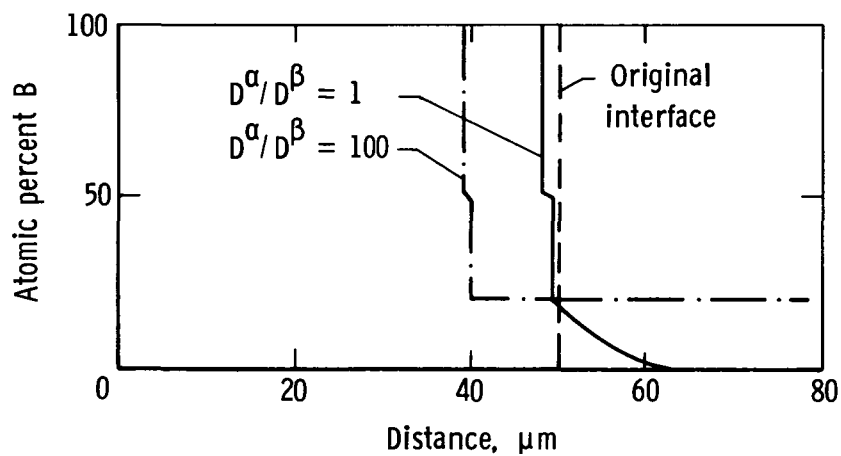


Figure 5.- Comparison of calculated and experimental interface migration data for planar W-Ni couples. $\bar{C}$ is given in atomic fraction of W.



(a) Normalized thickness of β - and γ -phases.



(b) Concentration profile at $\sqrt{t} = 50$.

Figure 6.- Effect of large D^α variations on (a) the change in normalized thickness of β - and γ -phases and (b) the concentration profiles for a cylindrical geometry specimen with $\bar{C} = 0.40$ atomic fraction of B.

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16. Abstract Numerical solutions were developed for treating one-dimensional transient diffusion in single-, two-, and three-phase binary alloy systems. These solutions are applicable for planar, cylindrical, or spherical geometries with any diffusion-zone size and any continuous variation (within a given phase) of the diffusion coefficient with concentration. Special techniques were included in the analyses to account for differences in molal volumes, initiation and growth of an intermediate phase (three-phase system), disappearance of a phase (two- and three-phase systems), and the presence of an initial composition profile in the specimen. A major improvement in solution accuracy was achieved in the two-phase analysis by employing a mass-conservation criterion to establish the location of the interface rather than the conventional interface-flux-balance criterion. In the three-phase analysis, computation time was minimized without sacrificing solution accuracy by treating the three-phase problem as a two-phase problem when the thickness of the intermediate phase was less than a preset small value. Three computer codes were developed to perform these analyses. The essential features of each code are discussed and information concerning the availability of these codes is included.					
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